

Isopentyl alcohol
123-51-3 | DTXSID3025469

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.25\text{e-}11$ cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: $8.48\text{e-}01$

Confidence level: $9.82\text{e-}01$

Nearest Neighbors from the Training Set

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Isopentyl alcohol

Measured: $1.31\text{e-}11$

Predicted: $1.25\text{e-}11$

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1-Hexanol

Measured: $1.25\text{e-}11$

Predicted: $1.24\text{e-}11$

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Pentan-2-ol

Measured: $1.18\text{e-}11$

Predicted: $1.20\text{e-}11$

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3-Pentanol

Measured: $1.22\text{e-}11$

Predicted: $1.20\text{e-}11$